Strain relaxation mechanism for hydrogen-implanted $Si_{1-x}Ge_x/Si(100)$ heterostructures

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A mechanism of strain relief of H^+ ion implanted and annealed pseudomorphic $Si_{1-x}Ge_x/Si(100)$ heterostructures grown by molecular beam epitaxy is proposed and analyzed. Complete strain relaxation was obtained at temperatures as low as 800 °C and the samples appeared free of threading dislocations within the SiGe layer to the limit of transmission electron microscopy analysis. In our model, H filled nanocracks are assumed to generate dislocation loops, which glide to the interface where they form strain relieving misfit segments. On the basis of this assumption, the conditions for efficient strain relaxation are discussed. © *2000 American Institute of Physics.* [S0003-6951(00)03424-0]

The implementation of a strain relieved $Si_{1-x}Ge_x$ buffer layer (SiGe BL) in a $Si_{1-x}Ge_x/Si(100)$ heterostructure offers a new degree of freedom in strain and band structure engineering. The tensile biaxial strain in a Si layer on a SiGe BL leads to a type II conduction band interface and enables the formation of a two-dimensional electron gas in a Si quantum well. Record electron mobilities have been measured in Si channels on SiGe BLs.[1,2] High frequency properties indicate the outstanding device potential of this material system.[3]

The state-of-the-art technique to produce high quality, SiGe BLs is the growth of several μm thick compositionally graded layers (up to $x \approx 0.3$),[4,5] which have, however, still threading dislocation (TD) densities on the order of $10^4-10^7\,cm^{-2}$. In addition, the several μm thick layers make the integration of SiGe devices on Si-based circuits difficult. Various strategies have been developed to reduce the TD density, including ion beam synthesis on silicon-on-insulator (SOI) structures,[6] growth on very thin SOI material,[7] and growth on low temperature Si or SiGe BLs.[8,9]

In this work, we have investigated the strain relaxation mechanism of molecular-beam-epitaxy grown, pseudomorphic $Si_{.85}Ge_{.15}$ heterostructures after H^+ implantation and annealing. Experimental results reported in previous publications demonstrated the success of this method up to Ge fractions of 22 at.%.[10] Here, the relaxation process of a $Si_{.85}Ge_{.15}/Si(100)$ structure was studied as a function of annealing temperature in order to reveal the underlying mechanisms and to clarify the conditions and limitations of the method.

A 250 nm thick, pseudomorphic $Si_{.85}Ge_{.15}$ layer on Si(100) was implanted with 25 keV H^+ ions at a dose of $3\times10^{16}\,cm^{-2}$ at room temperature. The implantation energy was chosen to create a defect region at the end-of-range about 50–100 nm below the SiGe/Si interface. The H^+ dose was about half of the dose used for Smart-Cut®.[11] Figure 1 shows two cross section transmission electron micrographs (XTEMs) of the sample after implantation and annealing at 600 and 800 °C for 7 min. Already at 600 °C, the SiGe layer recovered from the implantation damage and a defect region remains below the interface, where the formation of oblate nanocavities (platelets), preferentially oriented in the (100) plane, is observed. In addition, a high density of such cavities is found exactly at the interface. After annealing at

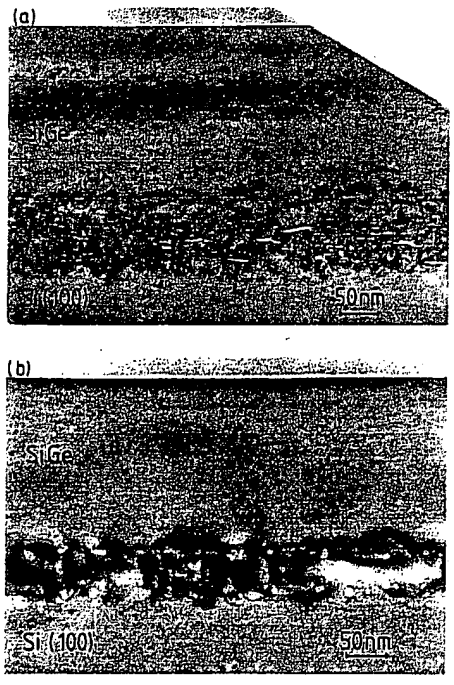

FIG. 1. XTEM micrographs of a 250 nm thick $Si_{.85}Ge_{.15}$ layer on Si(100) after H^+ implantation [25 keV, $3\times10^{16}\,cm^{-2}$] and thermal annealing at 600 °C (a) and 800 °C (b) for 7 min.

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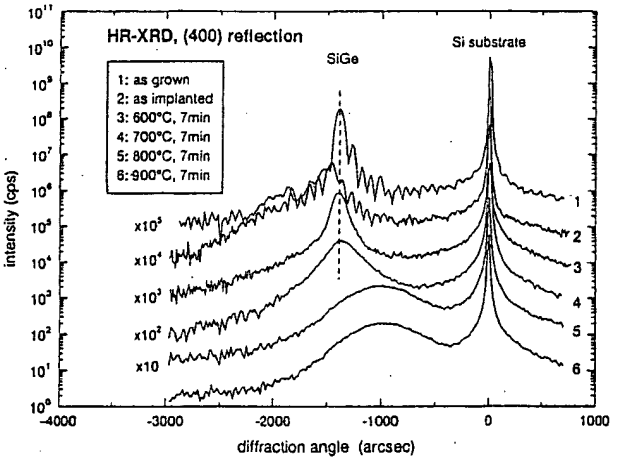

FIG. 2. XRD (400) rocking curve of a 250 nm thick $Si_{.85}Ge_{.15}$ layer on Si(100) after growth, after 25 keV H^+ ion implantation with a dose of 3×10^{16} cm^{-2}, and after subsequent thermal annealing at 600, 700, 800, and 900 °C for 7 min, respectively.

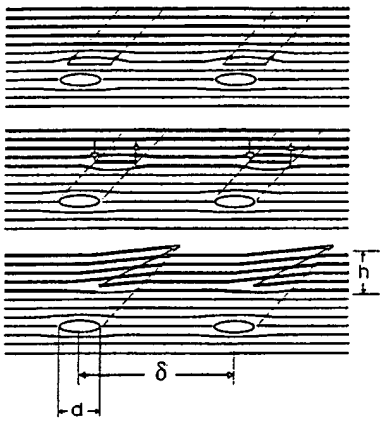

FIG. 3. Elementary steps in H induced strain relaxation schematically illustrated in a (010)-cut through a SiGe/Si(001) heterostructure [fat/thin lines indicate (001) lattice planes]. From top to bottom: (1) dislocation loops with [101]$a/2$ Burgers vector (arrows not drawn to scale) are generated by H-filled nanocracks, (2) loops glide in [101]-direction (dashed lines) to the SiGe epilayer where asymmetric forces (arrows) act on their segments, (3) segments on one (the right hand) side are pulled toward the surface where they form steps while the segments at the opposite side are hold in the interface where they form MD segments connected with the surface by TD segments (inclined lines).

800 °C, only spherical cavities remain at and below the interface. Strong strain contrast is observed between the interface and the cavities. A series of (400) x-ray rocking curves, shown in Fig. 2, indicate strain relaxation. After implantation, the SiGe layer peak showed additional strain caused by the incorporated H. After annealing at 600 °C the SiGe layer peak recovers to the initial position. At 700 °C the SiGe layer peak starts to broaden and to shift toward the peak of the Si substrate indicating the onset of strain relief. Nearly complete strain relaxation is achieved at 800 °C. In contrast, an unimplanted reference sample showed only a relaxation of 50% of its pseudomorphic strain even after annealing at 1100 °C. The misfit dislocation (MD) network in conventionally relaxed and H^+-implanted and annealed samples was studied by plane view TEM. The conventionally relaxed sample exhibits the well known MD network, whereas the H^+-implanted and annealed sample shows a much denser, irregular entanglement of dislocations. As shown already for a $Si_{.78}Ge_{.22}$ BL, no TDs were found by XTEM.[10]

In the following, we discuss the physical basis of strain relaxation by H^+ implantation and annealing. As in the conventional process of strain relaxation, four steps in the formation of MDs under the action of the plane stress associated with the misfit may be distinguished: (1) the formation (nucleation) of dislocation loops at the interface between the substrate and the epilayer or of half loops at the surface, (2) the growth of such loops through the epilayer until half loops, each consisting of a MD segment and two TDs are formed between the interface and the surface, (3) the motion of the two members of a pair of TDs in opposite directions resulting in an extension of the MD segment between them, and (4) the interaction of dislocation segments resulting in multiplication, blocking, or annihilation of TDs depending on the relation between their Burgers vectors.

In the conventional process of strain relaxation, the nucleation rate of dislocation loops is generally too low, leading to a rather inhomogeneous distribution of MDs and TDs. In particular, dislocation multiplication may result in piling up of TDs with equal Burgers vectors. Under such conditions, a TD is unlikely to find a partner of opposite sign for mutual annihilation within its interaction range, which is generally limited by the layer thickness. This is consistent with the experimental findings that, in conventional relaxation, the distance of TDs is frequently found to be of the order of the layer thickness.[12]

This essentially suggests an increase in the efficiency of the annihilation of TDs, even if it can only be achieved by increasing their primary density. A promising strategy for this consists of producing a relatively regular array of dislocation loops where each primary TD can find a partner for annihilation within its interaction range.

We are convinced that this is realized in strain relaxation with low residual TD densities achieved by H^+ implantation and annealing. This idea is supported by the observation that the characteristic distance of 50–100 nm in the MD network and in the cross-hatch pattern correlates well with the average distance between the oblate nanocavities induced by H^+ implantation.[10] Thus, the high density of cavities is considered here to provide a relatively regular array of dislocation sources required for the annihilation of TDs. The generation of dislocation loops by crack-like cavities formed by H or He ion implantation has been observed after He ion implantation into Si,[13] SiC,[14] and subsequent annealing.

From these findings, the following model for the elementary steps in our strain relaxation process emerges as illustrated in Fig. 3. At temperatures where H atoms are mobile in Si but self-diffusion is still negligible, H atoms cluster between (001) lattice planes and form nanocracks. The extremely high pressure within these cracks relaxes by the formation of (probably ⟨110⟩ square shaped) dislocation loops on (001) planes with ⟨101⟩$a/2$-type Burgers vectors. At temperatures where the loops become glissile, they glide, repelled by their native cracks and attracted by interfacial image forces, in appropriate {111} glide planes toward the interface. Since the Burgers vector of such a loop has an in-plane component, the plane stress in the SiGe layer associated with the misfit exerts asymmetric forces on the loop

segments according to the formula by Peach and Koehler.[15] For a [101]$a/2$ Burgers vector, for instance, the loop segments at the [100] oriented side (right hand side in Fig. 3) are pulled toward the surface where they form a step, while the segments at the opposite side are held in the interface where they form MD segments connected to the surface by two TD segments. The direct geometrical effect of this elementary step in strain relaxation is a thickening of the compressed layer in the region defined by the projection of the glide motion through the layer on the layer plane.

If the density of loops participating in this process is sufficiently high, virtually all TDs will find partners for mutual annihilation by combined climb-glide within their interaction range. Because of the existence of four equivalent Burgers vectors, however, loops with the same Burgers vector are generally not next nearest neighbors, but are separated by about twice the average loop spacing. Therefore, bypassing or cutting TDs with different Burgers vectors is generally necessary in an intermediate stage before annihilation can take place. The annihilation stage where the dislocation interaction dominates should be reached at the minimum motion of TDs necessary for annihilation in order to avoid a significant disturbance of the relatively regular original loop array and by this an increase in the probability for the occurrence of "lost" TDs without an annihilation partner in their range of interaction$<h$. This requirement implies a high density of loop sources.

Finally, we consider the conditions for efficient and healthy strain relaxation resulting from the above qualitative picture. Since the representative elastic modulus used cancels out (except Poisson's ratio) such conditions may be expressed as inequality relations between the original misfit strain ε_0 and the three characteristic length scales of the structure related to the lattice constant a or the Burgers vector b: (1) the (average) diameters d of the loops reaching the interface, (2) their distance δ, and (3) the layer thickness h. The average size and distance of the loops correspond to the ones of the crack-like cavities from which they originate.

For a loop segment to enter the epilayer the required force, exerted by the initial misfit stress field in the glide direction, must exceed the line tension force in the opposite direction. This condition may be expressed as a lower bound relation for ε_0 depending linearly on b/d. The condition for cutting two (unequal) TDs in an intermediate stage (where $\varepsilon_i \approx \varepsilon_0/2$) is analogous to, but more restrictive than, the one for the extension of a single TD. It may be expressed as a lower bound relation for ε_0 depending linearly on b/h. In the annihilation stage, the driving force for further extension of TDs must be smaller than the interaction forces between them. Estimates show that this implies almost complete strain relaxation $\varepsilon_a \rightarrow 0$. The condition for complete relaxation by a motion of TDs limited to about 2δ may be expressed as an upper bound relation for ε, depending on b/δ. Using the relevant expressions of dislocation theory[15] and taking the glide geometry properly into account, we express the conditions for entering the loop segment into the layer, for cutting unequal TDs, and for relaxation at minimum motion of TDs, respectively, as

$$\varepsilon_0 \geqslant 0.4b/d, \tag{1a}$$

$$\varepsilon_0 \geqslant b/h, \tag{1b}$$

$$\varepsilon_0 \leqslant b/\delta. \tag{1c}$$

The simultaneous fulfillment of conditions (1a) and (1c), and (1b) and (1c), respectively, requires

$$\delta \leqslant 2.5d, \tag{2a}$$

$$\delta \leqslant h. \tag{2b}$$

According to Eq. (2a), a high coverage of the interfacial region with loops and correspondingly with cracks is required for successful strain relaxation, i.e., a state close to the level $\delta \approx d$, where blistering or "smart cutting" would occur. Equation (2b) requires a high density of loops and correspondingly of cracks. Both conditions are consistent with our experimental findings. The most critical condition for high Ge concentrations ($\approx$30 at. %) with high misfit strains is expressed by Eq. (1c). It requires sufficiently small crack distances in the stage where loops become glissile.

In summary, we have shown that efficient and healthy strain relaxation of pseudomorphic SiGe/Si heterostructures by H^+ implantation and annealing with small residual dislocation densities may be attributed to the production of a very high density of dislocation loops at the interface punched out by H filled nanocracks. Specifically, the average distance between the nanocracks δ should meet the conditions $\delta \leqslant 2.5d$ (loop diameter d) and simultaneously $\delta \leqslant h$ (thickness h) meaning that for larger Ge fractions this length scale has to be further reduced by increasing the loop density. We are presently considering strategies in order to also apply the method for $Si_{1-x}Ge_x$ layers with Ge fractions $x>0.25$.

[1] K. Ismail, M. Arafa, K. L. Saenger, J. O. Chu, and B. S. Meyerson, Appl. Phys. Lett. **66**, 1077 (1995).
[2] G. Höck, M. Glück, T. Hackbarth, H.-J. Herzog, and E. Kohn, Thin Solid Films **336**, 141 (1998).
[3] M. Zeuner, T. Hackbarth, U. König, A. Gruhle, and F. Aniel, 57th *Annual Device Research Conference Digest*, University of California, Santa Barbara, 1999 (IEEE, New York 1999), Vol. 8393, p. 177.
[4] F. Schäffler, D. Többen, H.-J. Herzog, G. Abstreiter, and B. Holländer, Semicond. Sci. Technol. **7**, 260 (1992).
[5] E. A. Fitzgerald, Y. H. Xie, M. L. Green, D. Brasen, A. R. Kortan, J. Michel, Y. J. Mii, and B. E. Weir, Appl. Phys. Lett. **59**, 811 (1991).
[6] B. Holländer, S. Mantl, W. Michelsen, St. Mesters, A. Hartmann, L. Vescan, and D. Gerthsen, Nucl. Instrum. Methods Phys. Res. B **84**, 218 (1994).
[7] A. R. Powell, S. S. Iyer, and F. K. LeGoues, Appl. Phys. Lett. **64**, 1856 (1994).
[8] K. K. Linder, F. C. Zhang, J.-S. Rieh, P. Bhattacharya, and D. Houhgton, Appl. Phys. Lett. **70**, 3224 (1997).
[9] M. Bauer, K. Lyutovich, M. Oehme, E. Kasper, H.-J. Herzog, and F. Ernst, Thin Solid Films (to be published).
[10] S. Mantl, B. Holländer, R. Liedtke, S. Mesters, H. J. Herzog, H. Kibbel, and T. Hackbarth, Nucl. Instrum. Methods Phys. Res. B **147**, 29 (1999).
[11] M. Bruel, Nucl. Instrum. Methods Phys. Res. B **108**, 313 (1996).
[12] B. W. Dodson, J. Cryst. Growth **111**, 376 (1991).
[13] P. F. P. Fichtner, J. R. Kaschny, A. Kling, H. Trinkaus, R. A. Yankov, A. Mücklich, W. Skorupa, F. C. Zawislak, L. Amaral, M. F. da Silva, and J. C. Soares, Nucl. Instrum. Methods Phys. Res. B **136–138**, 460 (1998).
[14] J. Chen, P. Jung, and H. Trinkaus, Phys. Rev. Lett. **82**, 2709 (1999).
[15] J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw–Hill, New York, 1968).